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Some relations between rank, chromatic number and energy of graphs

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ABSTRACT

The energy of a graph G, denoted by $E(G)$, is defined as the sum of the absolute values of all eigenvalues of G. Let G be a graph of order n and $\mathrm{rank}(G)$ be the rank of the adjacency matrix of G. In this paper we characterize all graphs with $E(G) = \mathrm{rank}(G)$. Among other results we show that apart from a few families of graphs, $E(G) \geq 2\max(\chi(G), n - \chi(\overline{G}))$, where n is the number of vertices of G, $\overline{G}$ and $\chi(G)$ are the complement and the chromatic number of G, respectively. Moreover some new lower bounds for $E(G)$ in terms of $\mathrm{rank}(G)$ are given.

1. Introduction

Let G be a graph. Throughout this paper the *order* of G is the number of vertices of G. All the graphs that we consider in the paper are finite, undirected, and simple. If $\{v_1, \ldots, v_n\}$ is the set of vertices of G, then the *adjacency matrix* of G, $A = [a_{ij}]$, is an $n \times n$ matrix, where $a_{ij} = 1$ if v_i and v_j are adjacent and $a_{ij} = 0$ otherwise. Thus A is a symmetric matrix with zeros on the diagonal, and all eigenvalues of A are real. For a graph G, let $\mathrm{rank}(G)$ denote the rank of the adjacency matrix of G. The *spectrum* of graph G, $\mathrm{Spec}(G)$, is the set of the eigenvalues of A, denoted by $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$. We denote the *path* and the *complete graph* of order n by P_n and K_n, respectively. The *complete t-partite graph* is a graph whose vertices can be partitioned into t parts so that two vertices are adjacent if and only if they belong to different subsets of the partition. We denote the complete t-partite graph with parts of sizes $r_1, \ldots, r_t$ by $K_{r_1,\ldots,r_t}$. A *matching* of G is a set of mutually nonadjacent edges. A *perfect matching* of G is a matching which covers all vertices of G. For a graph G, *the chromatic number* of G, $\chi(G)$, is the minimum number of colors needed to color the vertices of G such that no two adjacent vertices have the same color.

The *Hückel molecular orbital*, HMO theory, is nowadays one of the most important fields of theoretical chemistry where graph eigenvalues occur. HMO theory deals with unsaturated conjugated molecules. The vertices of the graph associated with a given molecule are in one-to-one correspondence with the carbon atoms of the hydrocarbon system. Hückel theory in quantum chemistry ensures that the total π-electron energy of a conjugated hydrocarbon is simply the energy of the corresponding molecular graph.

The *energy* of a graph G is defined as the sum of the absolute values of all eigenvalues and denoted by $E(G)$. If $\lambda_1, \ldots, \lambda_s$ are all the positive eigenvalues of a graph G, then we have $E(G) = 2(\lambda_1 + \cdots + \lambda_s) = -2(\lambda_{s+1} + \cdots + \lambda_n)$. Recently much work on the energy of graphs appeared in [10,12,13,15,16].

2. Main results

First we state the following lemma.

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Lemma 1 ([5]). *If for every eigenvalue λ of a graph G, $\lambda \geq -1$, then G is a union of complete graphs.*

In [6], it is shown that for any graph G, $E(G) \geq \operatorname{rank}(G)$. Here we characterize all graphs G for which $E(G) = \operatorname{rank}(G)$.

Lemma 2. *Let G be a graph of order n. Then $E(G) \geq \operatorname{rank}(G)$ and equality holds if and only if $G = \frac{r}{2}K_2 \cup (n-r)K_1$ for some even positive integer r.*

Proof. Assume that $\lambda_1, \ldots, \lambda_r$ are all the non-zero eigenvalues of G. Let $\lambda^{n-r}(\lambda^r + a_1\lambda^{r-1} + \cdots + a_r)$ be the characteristic polynomial of G, where a_r is a nonzero integer. Then the arithmetic-geometric inequality implies that

$$\frac{|\lambda_1| + \cdots + |\lambda_r|}{r} \geq \sqrt[r]{|\lambda_1| \cdots |\lambda_r|} = \sqrt[r]{|a_r|} \geq 1. \tag{1}$$

Thus $E(G) \geq \operatorname{rank}(G)$. If $G = \frac{r}{2}K_2 \cup (n-r)K_1$, obviously $E(G) = \operatorname{rank}(G)$. Conversely, suppose that $E(G) = \operatorname{rank}(G)$. So equality holds in (1), that is $|\lambda_1| = \cdots = |\lambda_r| = 1$. Now, by Lemma 1, $G = \frac{r}{2}K_2 \cup (n-r)K_1$. □

In [2], it is shown that the energy of a connected graph with at least two vertices is greater than 1. In the following we improve this lower bound.

Theorem 1. *For any connected graph G apart from K_1 and $K_{1,i}$, $1 \leq i \leq 3$, $E(G) \geq 4$.*

Proof. We may assume that G has at least four vertices. Clearly, $\operatorname{rank}(G) \geq 2$. If $\operatorname{rank}(G) = 2$, it is shown in [1] that G is a complete bipartite graph. So G is $K_{r,s}$, $rs \geq 4$, and $E(G) \geq 2\sqrt{rs} \geq 4$. If $\operatorname{rank}(G) = 3$, then G has three non-zero eigenvalues. Also G has exactly one positive eigenvalue; otherwise, the sum of the eigenvalues of G is not zero because $\lambda_1(G)$ has the greatest absolute value. Hence by Theorem 6.7 of [5, p. 163], G is a complete multipartite graph. Since the rank of a complete t-partite graph is t, G is a complete 3-partite graph. Therefore G has K_3 as an induced subgraph. Thus by Interlacing Theorem (Theorem 0.10 of [5]) $E(G) \geq E(K_3) = 4$. If $\operatorname{rank}(G) \geq 4$, then by Lemma 2, $E(G) \geq 4$. □

Theorem 2. *If G is a connected bipartite graph of rank r, then $E(G) \geq \sqrt{(r+1)^2 - 5}$.*

Proof. Let $\lambda_1, \ldots, \lambda_s$ be the positive eigenvalues of G, where $s = r/2$. Then

$$E^2(G) = \left(2\sum_{i=1}^{s} \lambda_i\right)^2 = 4\left(\sum_{i=1}^{s} {\lambda_i}^2 + \sum_{i \neq j} \lambda_i\lambda_j\right) = 4\left(m + s(s-1)a\right),$$

where m is the number of edges in G and a is the arithmetic mean of $\{\lambda_i\lambda_j\}_{i\neq j}$. The geometric mean of $\{\lambda_i\lambda_j\}_{i\neq j}$ is

$$\left(\prod_{i\neq j} \lambda_i\lambda_j\right)^{(s(s-1))^{-1}} = k^{1/s},$$

where $k = {\lambda_1}^2 \cdots {\lambda_s}^2$. Since G is connected, $m \geq r - 1$. Note that $k \geq 1$. So we have

$$E(G) \geq \sqrt{4m + r(r-2)\sqrt[r]{k^2}} \geq \sqrt{(r+1)^2 - 5}. \quad \square$$

The proof of the following lemma is easy and we leave it to the reader.

Lemma 3. *If T is a tree with no perfect matching and isolated vertex, then T has at least two maximum matchings.*

The following lemma is an immediate consequence of Harary's Theorem, see [3, p. 44].

Lemma 4. *The number of maximum matchings of a tree is equal to the product of its non-zero eigenvalues.*

Corollary 1. *If T is a tree with no perfect matching, then the product of its non-zero eigenvalues is at least 2.*

Theorem 3. *Let G be a bipartite graph with at least 4 vertices. If G is not full rank, then $E(G) \geq 1 + \operatorname{rank}(G)$.*

Proof. Without loss of generality, we may assume that G is a connected graph. From the proof of Theorem 2, we have $E(G) \geq \sqrt{4m + r(r-2)\sqrt[r]{k^2}}$, where $r = \operatorname{rank}(G)$ and $k = \lambda_1^2 \cdots \lambda_s^2$ and $\lambda_1, \ldots, \lambda_s$ are positive eigenvalues of G, $s = r/2$. If G is a tree, then by Theorem 8.1 of [5], G has no perfect matching. Thus Corollary 1 implies that $k \geq 2$. Hence $E(G) \geq \sqrt{4(n-1) + r(r-2)\sqrt[r]{4}}$. Note that G is not full rank. So we have $E(G) \geq \sqrt{4r + r(r-2)\sqrt[r]{4}}$. Note that if $r \geq 3$, then $\sqrt[r]{4} > \exp(1/r) > 1 + \frac{1}{r} \geq 1 + \frac{1}{r(r-2)}$. Thus if $r \geq 3$, $E(G) > \sqrt{4r + r(r-2) + 1} = r + 1$. If $r = 2$, then by Theorem 1 we are done. If G is not a tree, then since G is not full rank, we find, $m \geq n \geq r + 1$, and the proof is complete. □

Now, we would like to obtain some lower bounds for $E(G)$ in terms of the chromatic number of G and the chromatic number of $\overline{G}$.

Theorem A (*Theorem 2.30 of [7]*). *For any graph G, $n - \chi(\overline{G}) \leq \lambda_1 + \cdots + \lambda_{\chi(\overline{G})}$.*

By Theorem A, we have the following result.

Theorem 4. *For every graph G, $E(G) \geq 2(n - \chi(\overline{G}))$.*

Remark 1. A well-known theorem of Nordhaus and Gaddum [11] states that for every graph G of order n, $\chi(G) + \chi(\overline{G}) \leq n + 1$. The graphs attaining equality in the Nordhaus–Gaddum Theorem were characterized by Finck [8], who proved that there are exactly two types of such graphs, the types (a) and (b) defined as follows.

(i) A graph G is of type (a) if it has a vertex v such that $V \setminus \{v\}$ can be partitioned into subsets K and S with the properties that $K \cup \{v\}$ induces a clique of G and $S \cup \{v\}$ induces an independent set of G (adjacency between K and S is arbitrary). Note that if G is of type (a), then so does its complementary graph $\overline{G}$.
(ii) A graph G is of type (b) if it has a subset C of five vertices such that $V \setminus C$ can be partitioned into subsets K and S with the properties that K induces a clique, S induces an independent set, C induces a 5-cycle, and every vertex of C is adjacent to every vertex of K and to no vertex of S (adjacency between K and S is arbitrary). Note that if G is of type (b), then so is its complementary graph.

If we omit a perfect matching from the complete graph K_{2n}, the resulting graph is called *cocktail party* and denoted by $CP(n)$. For any graph G with vertices $\{v_1, \ldots, v_n\}$, and any non-negative integers $a_1, \ldots, a_n$, we construct the *generalized line graph* $L(G; a_1, \ldots, a_n)$ as follows:

The vertex set is the union of the vertex sets of $L(G), CP(a_1), \ldots, CP(a_n)$, and the edge set is the union of the edge sets, together with edges joining all vertices of $CP(a_i)$ to every vertex of $L(G)$ corresponding to an edge of G containing v_i, for $1 \leq i \leq n$.

Denote by $A_{n,t}$ for $1 \leq t \leq n-1$ the graph obtained by joining a new vertex to t vertices of the complete graph K_n. If we add two pendant vertices to a common vertex of K_n, then the resulting graph has order $n+2$ and we denote it by B_n. For the proof of the next theorem we need the following interesting result due to Wilf, see [3, p. 55].

Lemma 5. *For any graph G, $\chi(G) \leq \lambda_1(G) + 1$, where $\lambda_1(G)$ denotes the largest eigenvalue of G.*

Theorem 5. *Let G be a graph. Then $E(G) < 2\chi(G)$ if and only if G is a union of some isolated vertices and one of the following graphs:*

(i) *the complete graph K_n;*
(ii) *the graph B_n;*
(iii) *the graph $A_{n,t}$ for $n \leq 7$, except when $(n, t) = (7, 4)$, and for $n \geq 8$ with $t \in \{1, 2, n-1\}$;*
(iv) *a triangle with two pendant vertices adjacent to different vertices (see the graph H_5 in Fig. 2).*

Proof. First we show that the graphs stated in the theorem satisfy $E(G) < 2\chi(G)$. The assertion is clear for complete graphs. The characteristic polynomial of B_n (see [5, p. 159]) is

$$\lambda(\lambda+1)^{n-2}[(\lambda^2-2)(\lambda-n+2)+\lambda(\lambda-n+1)(\lambda+1)+\lambda^2(\lambda-n+2)].$$

Therefore B_n has at least $n-2$ eigenvalues -1. By Lemma 1 we find $\lambda_{n+2} < -1$, so by Theorem 6.7 of [5], B_n has exactly two positive eigenvalues. This implies that $E(B_n) = -2(\lambda_{n+2} - n + 2)$ since the sum of eigenvalues of any graph is zero. On the other hand the characteristic polynomial of B_n is $\lambda(\lambda+1)^{n-2}f(\lambda)$, where $f(\lambda) = \lambda^3 + (2-n)\lambda^2 - (1+n)\lambda + 2n - 4$. It is not hard to see that $f(\lambda) < f(-2) = -2$ for any $\lambda < -2$. Therefore all eigenvalues of B_n are more than -2. Thus $E(B_n) = -2(\lambda_{n+2} - n + 2) < 2n = 2\chi(B_n)$.

A calculation shows that for $n \leq 7$, $E(A_{n,t}) < 2n = 2\chi(A_{n,t})$ except $E(A_{7,4}) = 14$. So we may assume that $n \geq 8$. The graph K_n has $n-1$ eigenvalues -1, therefore by Interlacing Theorem, the graph $A_{n,t}$ has at least $n-2$ eigenvalues -1. On the other hand the graphs $A_{n,1}$ and $A_{n,2}$ are not complete multipartite graphs, so they have at least two positive eigenvalues. Then again Interlacing Theorem implies that these two graphs have exactly two positive eigenvalues. The graphs $A_{n,1}$ and $A_{n,2}$ are line graphs, and $A_{n,n-1} = L(K_{1,n-1}; 1, 0, \ldots, 0)$, where the vertex v_1 in $K_{1,n}$ is the vertex with maximum degree. Hence their eigenvalues are at least -2 and Theorem 1.6 of [4] shows that $\lambda_{n+1} > -2$. Thus $E(A_{n,t}) = -2(\lambda_{n+1} - n + 2) < 2n$ for $t = 1, 2$. The graph $A_{n,n-1}$ has a zero eigenvalue, and in the same way we find that $E(A_{n,n-1}) < 2n$. Now, let $2 < t < n-1$. We claim that the graph $A_{n,t}$ cannot be a generalized line graph. For any $l \geq 2$, $CP(l)$ has C_4 as an induced subgraph and if $A_{n,t}$ is a generalized line graph, then we conclude that $A_{n,t} = L(K_{1,n-1}; 1)$. Clearly, $A_{n,t}$ is not isomorphic to $L(K_{1,n-1}; 1)$. Thus by Exercise 14 of [9, p. 278], $\lambda_{n+1} \leq -2$. Hence $E(A_{n,t}) \geq 2n$. Finally for the graph H_5 (see Fig. 2) by an easy computation we see $E(H_5) < 2\chi(H_5)$ (see [14]).

Now, we show that apart from exceptional cases of the theorem, for any graph G, $E(G) \geq 2\chi(G)$. If G has two non-trivial components, then G has $2K_2$ as an induced subgraph. Hence Interlacing Theorem (Theorem 0.10 of [5]) and Lemma 5 imply that $E(G) \geq 2(\lambda_1 + \lambda_2) \geq 2(\lambda_1 + 1) \geq 2\chi(G)$. Since isolated vertices do not contribute to the energy and the chromatic

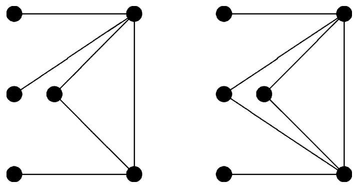

Fig. 1. The graphs H_1 and H_2.

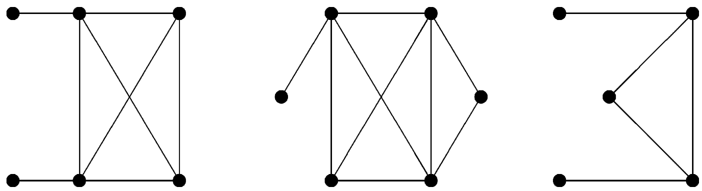

Fig. 2. The graphs H_3, H_4, and H_5.

number, we may assume that G is connected. By Remark 1, we have $\chi(G) + \chi(\overline{G}) \le n + 1$. If $\chi(G) + \chi(\overline{G}) \le n$, then we are done by Theorem 4. So we let $\chi(G) + \chi(\overline{G}) = n + 1$. In this case G is either of type (a) or of type (b). If G is of type (b), then G has C_5 as an induced subgraph. Therefore $\lambda_2(G) + \lambda_3(G) \ge \lambda_2(C_5) + \lambda_3(C_5) > 1$. Note that $\lambda_3(C_5) > 0$. Thus by Lemma 5 we have

$$E(G) \ge 2(\lambda_1 + \lambda_2 + \lambda_3) > 2(1 + \lambda_1) \ge 2\chi(G).$$

Thus one may assume that G is of type (a). For simplification let $|K| = t$, where K is a complete subgraph of G defined in Remark 1. It is easily seen that $\chi(G) = t + 1$. Clearly, K_{t+1} is an induced subgraph of G. We know that K_{t+1} has one eigenvalue t and t eigenvalues -1. So by Interlacing Theorem, G has at least t eigenvalues which are at most -1. If G has an induced subgraph with at least one eigenvalue λ such that $\lambda \le -2$, then the sum of all negative eigenvalues of G is less than $-(t-1) - 2 = -t - 1$. Thus $E(G) \ge 2t + 2 = 2\chi(G)$.

Therefore we may assume that every eigenvalue of each induced subgraph of G is more than -2. This implies that G has no $K_{1,4}$ as an induced subgraph. Hence every vertex of K is adjacent to at most two vertices of S.

First suppose that there is a vertex $a \in K$ which is adjacent to two vertices $\{x, y\} \subseteq S$. If $|S| \ge 3$, then there exists a vertex $z \in S \setminus \{x, y\}$ such that z is adjacent to a vertex $b \in K$ and $b \ne a, v$, where v is the vertex given in Remark 1. Thus G has either H_1, or H_2 as an induced subgraph (see Fig. 1).
We have (see [14]) $\lambda_6(H_1) < -1.8$, $\lambda_5(H_1) < -1.3$, and $\lambda_6(H_2) < -1.7$, $\lambda_5(H_2) < -1.6$. Since G has at least t eigenvalues which are at most -1, the sum of all negative eigenvalues of G is less than $-(t-2)-3 = -t-1$. Thus $E(G) \ge 2t+2 = 2\chi(G)$. If $|S| = 2$, there exist two cases: (1) $G = B_{n-2}$; (2) G has either $K_{1,1,3}$ or H as an induced subgraph, where H is the graph obtained by removing one of the pendant vertices of H_2. If (1) is the case, then $E(G) < 2\chi(G)$. If (2) is the case, since $\lambda_5(K_{1,1,3}) = -2$, $\lambda_5(H) < -1.74$, and $\lambda_4(H) < -1.27$, as before we conclude that $E(G) \ge 2\chi(G)$.

Now, suppose that every vertex in K is adjacent to at most one vertex of S. If $|S| \ge 2$ and $|K| \ge 3$, then G has an induced subgraph isomorphic to H_3 or H_4.

The graph H_3 has two eigenvalues one of which is less than -1.39 and the other one is less than -1.61. Also H_4 has two eigenvalues one of which is less than -1.3 and the other one is less than -1.7, see [14]. Thus $E(G) \ge 2\chi(G)$. It remains to consider the case $|S| \le 1$ or $|K| \le 2$. If $|S| = 0$, then $G = K_n$. If $|S| = 1$, then $G = A_{n,t}$ for some t. If $|K| \le 2$, then $|S| \le 2$. It can be easily checked that G is one of the graphs $B_1 = K_{1,2}, A_{3,1}, A_{3,2}, H_5$ or K_i, $i = 1, 2, 3$. □

Let G be a connected graph of order n. The following corollary shows that either the graph G, or $\overline{G}$ has energy at least n. Compare with Corollary 5.2 of [10] which states that if G has no zero eigenvalue, then $E(G) \ge n$.

Corollary 2. *Let G be a graph of order $n \ge 3$. If G or $\overline{G}$ is neither a complete graph nor one of the graphs $A_{k,k-1}$, B_1, B_2, and $A_{3,1}$, then $E(G) + E(\overline{G}) \ge 2n$.*

Proof. If $\overline{G}$ is not one of the graphs described in Theorem 5, then $E(\overline{G}) \ge 2\chi(\overline{G})$ and the corollary follows from Theorem 4. If $G = H_5$, then $E(G) + E(\overline{G}) > 10$. If G is a complete graph, B_1, B_2, or $A_{3,1}$, it is easily seen that $E(G) + E(\overline{G}) < 2n$. If $G = A_{k,k-1}$, then $\overline{G} = K_2 \cup (k-1)K_1$. Hence $E(A_{k,k-1}) + E(\overline{A_{k,k-1}}) < 2k + 2 = 2n$. To complete the proof, it is enough to show that the theorem holds for B_k, $k \ge 3$ and $A_{k,t}$ for $k \ge 4$, and $t = 1, 2$. The graph B_k has $k - 2$ eigenvalues -1, and $\lambda_n(B_k) \le \lambda_6(B_4) < -1.8$. So $E(B_k) > 2(k - 0.2)$. On the other hand $K_{1,1,2}$ is an induced subgraph of $\overline{B_k}$. Therefore $E(\overline{B_k}) \ge E(K_{1,1,2}) > 5$ and so $E(B_k) + E(\overline{B_k}) \ge 2(k + 2)$.

The graph $A_{k,t}$ has $k-1$ eigenvalues -1 and $\lambda_n(A_{k,1}) \le \lambda_5(A_{4,1}) < -1.5$, so $E(A_{k,1}) > 2k-1$. Also $\lambda_n(A_{k,2}) \le \lambda_5(A_{4,2}) < -1.68$, hence $E(A_{k,2}) > 2k - 0.64$. Now, the facts $E(\overline{A_{k,1}}) \ge E(K_{1,3}) > 3.4$ and $E(\overline{A_{k,2}}) \ge E(K_{1,2}) > 2.8$ complete the proof. □

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